

CONCRETE MIXTURE OPTIMIZATION USING STATISTICAL MIXTURE DESIGN METHODS

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ABSTRACT

The optimization of mixture proportions for high-performance concretes, which contain many constituents and are often subject to several performance constraints, can be a difficult and time-consuming task. Statistical experiment design and analysis methods have been developed specifically for the purpose of optimizing mixtures, such as concrete, in which the final product properties depend on the relative *proportions* of the components rather than their absolute amounts. Although mixture methods have been used in industry to develop products such as gasoline, metal alloys, detergents and foods, they have seen little application in the concrete industry. This paper describes an experiment in which a statistical mixture experiment was used to optimize a six-component concrete mixture subject to several performance constraints. The experiment was performed in order to assess the usefulness of this technique for high performance concrete mixture proportioning in general.

INTRODUCTION

In the simplest case, portland cement concrete is a mixture of water, portland cement, fine aggregate, and coarse aggregate. Additional components, such as chemical admixtures (air entraining agents, superplasticizers) and mineral admixtures (coal fly ash, silica fume, blast furnace slag), may be added to the basic mixture to enhance certain properties of the fresh or hardened concrete. High-performance concrete mixtures, which may be required to meet several performance criteria (e.g., compressive strength, elastic modulus, rapid chloride permeability) simultaneously, typically contain at least six components.

In a recent paper, Rougeron and Aitcin¹ stated that, "The optimization of the composition of a high performance concrete (HPC) is at present more of an art than a science...." Even for conventional concrete mixes, the American Concrete Institute (ACI) guideline document for mix proportioning² provides a method for proportioning one mix, but it does not provide a procedure for finding the proportions which provide the best settings to meet a number of performance criteria simultaneously. The recent ACI guideline document for proportioning high-strength concrete containing fly ash³ also does not provide a means for optimizing mixtures. The selection of mix proportions for a conventional concrete mix, with strength as the primary criterion, may not require a significant number of trial batches to find an appropriate mix. However, for a concrete mixture containing six or more components which must satisfy several performance constraints, trial and error or "one factor at a time" approaches sufficient for a conventional mix will be inefficient and costly. More importantly, they may not provide the best combination of materials at minimum cost.

In this study, a statistically designed mixture experiment was used to identify the best factor settings for optimizing properties of high performance concrete. In a mixture experiment, the total amount (mass or volume) of the mixture is fixed and the factors or component settings are proportions of the total amount. For concrete, the sum of the volume fractions is constrained to sum to one, as in the ACI mix design approach². Because the volume fractions must sum to unity, the component variables in a mixture experiment are not independent.

One viable experiment design option for concrete mixtures^{1,4} is the factorial design, in which the q mixture components are reduced to $q-1$ independent factors by taking the ratio of two components. There are advantages and disadvantages to both the mixture and factorial approaches. For example, the experimental region of interest is defined more naturally in the mixture experiment approach, but the analysis of such experiments is more complicated. The factorial (independent variables) approach permits the use of classical factorial and response surface designs^{5,8}, but has the undesirable feature that the experimental region changes depending on how the q mixture components are reduced to $q-1$ independent factors.

Because mixture experiments have not been readily used in the concrete industry, the utility of this approach for optimizing concrete properties was investigated. An experiment was designed to find the optimum proportions for a concrete mix meeting the following conditions: 50 to 100 mm (2 to 4 in) slump for the fresh concrete, 1-day target compressive strength of 22.06 MPa (3200 psi), 28-day target compressive strength of 51.02 MPa (7400 psi), target 42-day "rapid chloride" (ASTM C1202) test (RCT) measurement less than 700 coulombs, and minimum cost (dollars per m³). The materials (components) used included water, cement, microsilica (silica fume), high-range water reducing admixture (HRWRA), coarse aggregate, and fine aggregate.

EXPERIMENT DESIGN

Background on Mixture Experiments

As a simple (hypothetical) example of a mixture experiment, consider concrete as a mixture of three components: water (x_1), cement (x_2), and aggregate (x_3), where each x_i represents the volume fraction of a component. Assume the coarse-to-fine aggregate ratio is held fixed. The volume fractions of these components sum to one,

$$x_1 + x_2 + x_3 = 1 \quad (1)$$

and the region defined by this constraint is the regular triangle (or simplex) shown in Figure 1. The axis for each component x_i extends from the vertex it labels ($x_i = 1$) to the midpoint of the opposite side of the triangle ($x_i = 0$). The vertex represents the pure component. For example, the vertex labelled x_1 is the pure water "mixture" with $x_1 = 1$, $x_2 = 0$, and $x_3 = 0$, or (1,0,0). The coordinate where the three axes intersect is (1/3,1/3,1/3) and is called the centroid.

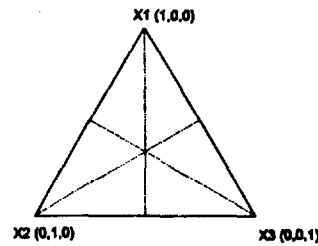


Figure 1. Experimental region for three component mixture

A good experiment design for studying properties over the entire region of a three-component mixture would be the simplex-centroid design shown in Figure 2. This example is included for illustrative purposes only, since much of this region does not represent feasible concrete mixtures. The points shown in Figure 2 represent mixtures included in the experiment. This design includes all vertices, midpoints of edges, and the overall centroid. All properties of interest would be measured for each mix in the design and modeled as a function of the components.

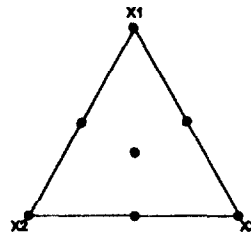


Figure 2. Layout of experiment design for three component simplex-centroid mixture

Typically, polynomial functions are used for modeling, but other functional forms can be used as well. For three components, the linear polynomial for a response y is

$$y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + e \quad (2)$$

where the b_i^* are constants and e , the random error term, represents the combined effects of all variables not included in the model. This model is typically reparameterized in the form

$$y = b_1x_1 + b_2x_2 + b_3x_3 + e \quad (3)$$

using $b_0^* = b_0^*(x_1 + x_2 + x_3)$ and is called the Scheffé⁹ linear mixture polynomial. Similarly the quadratic polynomial

$$y = b_0^* + b_1^*x_1 + b_2^*x_2 + b_3^*x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + b_{11}x_1^2 + b_{22}x_2^2 + b_{33}x_3^2 + e \quad (4)$$

is reparameterized as

$$y = b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + e \quad (5)$$

using $x_1^2 = x_1(1 - x_2 - x_3)$, $x_2^2 = x_2(1 - x_1 - x_3)$, $x_3^2 = x_3(1 - x_1 - x_2)$.

Since feasible concrete mixes do not exist over the entire region shown in Figure 1, a meaningful subregion of the full simplex must be defined by constraining the component proportions. An example of a possible subregion for the three component example is shown in Figure 3. It is defined by the following volume fraction constraints (x_1 = water, x_2 = cement, x_3 = aggregate):

$$0.15 \leq x_1 \leq 0.25$$

$$0.10 \leq x_2 \leq 0.20$$

$$0.60 \leq x_3 \leq 0.70$$

In this case the simplex designs are generally no longer appropriate and other designs¹⁰ are used. These designs typically include the extreme vertices of the constrained region and a subset of the remaining centroids (e.g., centers of edges, faces, etc.).

Experiment Design for the Six-Component Study

Selection of proportions and constraints - The proportions for the six-component mixture experiment were initially selected in terms of volume fraction and converted to weights for batching. The minimum and maximum levels of each component were chosen based on typical volume fractions for non air-entrained concrete¹¹ with the constraint that the volume

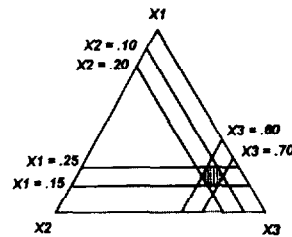


Figure 3. Example of constrained experimental region

fractions sum to unity. In addition to the individual constraints on each component, the paste fraction of the concrete (water, cement, microsilica, and HRWRA) was required to range from 25 to 35 percent by volume. Although air is incorporated into concrete during mixing, it is not an initial component and therefore was not considered to be a component of the mixture. Ignoring the air content as a mix component affects yield calculations, but these are not important for the small trial batches and can be adjusted later after a final mix is selected.

Table 1 – Mixture Components and Volume Fraction Ranges

Component	ID	Minimum volume fraction	Maximum volume fraction
Water	x_1	.16	.185
Cement	x_2	.13	.15
Microsilica	x_3	.013	.027
HRWRA	x_4	.0046	.0074
Coarse Aggregate	x_5	.40	.4424
Fine Aggregate	x_6	.25	.2924

The six components and the final ranges of their volume fractions for this experiment are shown in Table 1. The volume fractions were converted to corresponding weights using the specific gravities and percent solids (where applicable) obtained from laboratory testing or from the material supplier.

Experiment Design Details - The selection of an appropriate experiment design depends on several criteria, such as ability to estimate the underlying model, ability to provide an estimate of repeatability, and ability to check the adequacy of the fitted model. These issues are addressed below.

The “best” experiment design depends on the choice of an underlying model which will adequately explain the data. For this experiment, the following quadratic Scheffé polynomial was chosen as a reasonable model for each property as a function of the six components:

$$y = b_1x_1 + \dots + b_6x_6 + b_{12}x_1x_2 + \dots + b_{56}x_5x_6 + e \quad (6)$$

This model is an extension of Equation 5 for the six component case. Since there are 21 coefficients in the model, the design must have at least 21 runs (21 distinct mixes) to estimate these coefficients. In addition to the 21 required runs, seven additional runs (distinct mixes) were included to check the adequacy of the fitted model, and five mixes were replicated to provide an estimate of repeatability allowing us to test the statistical significance of the fitted coefficients. Finally, a single mix was replicated during each

week of the experiment to check statistical control of the fabrication and measurement process. In all, a total of 36 mixes were planned.

Commercially available computer software for experiment design was used for design and analysis of the experiment. The program selected thirty-six points from a list of candidate points that is known to include the best points for fitting a quadratic polynomial. A modified-distance design⁶ was chosen to ensure that the design selected could estimate the quadratic mixture model while spreading points as far away as possible from one another.

Table 2 summarizes the mixes used in the experiment. The run order was randomized to reduce the effects of extraneous variables not explicitly included in the experiment. The first three mixes were repeated at the end of the program because an incorrect amount of water was used in batching them. The test results from the incorrectly batched mixes were not included in the subsequent analysis. A total of 39 batches were prepared, from which 36 sets of test results were analyzed.

SPECIMEN FABRICATION AND TESTING

The materials used in this study included a Type I/II Portland cement, tap water, #57 crushed limestone coarse aggregate, natural sand, microsilica (in slurry form), and a naphthalene-sulfonate based superplasticizer (ASTM C494 Type F/G). Thirty-nine batches of concrete, each approximately $.04 \text{ m}^3$ (1.5 ft^3) in volume, were prepared over a four-week period. A rotating-drum mixer with a 0.17 m^3 (6.0 ft^3) capacity was used to mix the concrete.

Each batch included sufficient concrete for two slump tests, two fresh air content (ASTM C231) tests, two unit weight tests, and ten 100 mm by 200 mm (4 in by 8 in) cylinders. The cylinders were fabricated in accordance with ASTM C192. In order to obtain adequate consolidation, cylinders for concretes with slumps less than 50 mm (2 in) were vibrated on a vibrating table; otherwise, the cylinders were rodded. The cylinders were covered with plastic and left in the molds for 22 hours, after which they were stripped and placed in limewater-filled curing tanks for moist curing at $23 \pm 2^\circ\text{C}$ ($73 \pm 3^\circ\text{F}$).

Compressive strength tests (ASTM C39) were conducted on the cylinders at the ages of one day and 28 days. In most cases, three cylinders were tested for each age. A fourth test was performed in some cases if one result was significantly lower or higher than the others. Before testing, the cylinder ends were ground parallel to meet the ASTM C39 requirements using an end-grinding machine designed for this purpose. The three remaining cylinders from each batch were used for "rapid chloride" testing according to ASTM C1202. Three specimens (50 mm (2 in) thick slices taken from the middles of the concrete cylinders) were tested at an age of 42 days.

Table 2 - Summary of mix proportions (per cubic meter of concrete)

Design ID	Run Order	Water	Cement	Silica fume	HRWRA	Coarse aggregate (dry)	Fine aggregate (dry)	w/(c+sf)
		(kg)	(kg)	(kg)	(l)	(kg)	(kg)	
5(r)	7, 22	122.3	312.9	45.4	3.52	867.6	506.3	0.35
11(r)	6, 23	141.4	312.9	21.9	3.52	845.3	506.3	0.43
13	15	122.3	312.9	21.9	3.52	810.1	592.2	0.37
15	2*, 38	126.6	361.1	45.4	5.66	810.1	506.3	0.32
16	8	122.3	312.9	21.9	3.52	895.9	506.3	0.37
20(r)	13, 34	141.4	312.9	21.9	3.52	810.1	541.8	0.43
22	4	141.4	354.8	21.9	3.52	810.1	506.3	0.38
28	16	122.3	312.9	45.4	3.52	810.1	563.8	0.35
37	30	122.3	337.0	45.4	5.66	810.1	537.9	0.33
38(r)	3*, 26, 39	135.0	341.1	45.4	3.52	810.1	506.3	0.36
48	28	131.8	312.9	21.9	5.66	810.1	561.2	0.41
63	27	131.8	312.9	45.4	5.66	836.6	506.3	0.38
65	31	122.3	337.0	45.4	5.66	841.7	506.3	0.33
66	25	122.3	312.9	45.4	5.66	836.0	532.2	0.35
70	29	122.3	361.1	21.9	4.59	810.1	548.8	0.33
71(r)	5, 35	122.3	361.1	21.9	5.66	829.9	526.1	0.33
78	11	141.4	312.9	45.4	5.66	810.7	506.9	0.41
87	24	122.3	312.9	21.9	3.52	853.0	549.2	0.37
89	19	122.3	337.0	21.9	3.52	810.1	571.9	0.35
91	9	141.4	312.9	21.9	5.66	824.9	521.1	0.43
98	17	122.3	337.0	21.9	3.52	875.7	506.3	0.35
101	10	130.8	361.1	21.9	3.52	832.8	506.3	0.35
103	14	122.3	361.1	21.9	4.59	852.6	506.3	0.33
110	21	130.8	361.1	21.9	3.52	810.1	529.0	0.35
116	33	131.8	312.9	45.4	5.66	810.1	532.8	0.38
123	36	122.3	337.0	33.6	4.59	834.4	530.6	0.34
127(c)	1*, 12, 18, 32, 37	131.5	335.8	21.9	4.59	829.9	526.1	0.38
163	20	126.6	323.3	27.8	5.12	857.5	513.6	0.37

Notes: 1 l = 33.81 oz., 1 kg = 2.2046 lb.
(r) indicates replicated mix
(c) indicates control mix
* indicates mix which was repeated due to incorrect batching

RESULTS AND ANALYSIS

The average values for slump, 1-day strength, 28-day strength, rapid chloride test measurement (coulombs) for each batch are shown in Table 3, along with the estimated cost per cubic yard of concrete. The cost of each batch was calculated from the mix

Table 3 – Test Results and Costs

Design ID	Run	Slump (mm)	1-day str (MPa)	28-day str (MPa)	42-day RCT (coulombs)	Cost (\$/ m³)
22	4	67	21.5	48.2	1278	95.18
71	5	57	27.0	55.2	862	102.22
11	6	102	16.8	48.5	1162	91.32
5	7	13	22.4	48.5	387	118.85
16	8	35	21.6	53.1	776	92.20
91	9	200	16.8	60.4	1027	96.89
101	10	22	26.6	53.6	744	96.24
78	11	127	19.2	51.7	492	123.56
127	12	99	21.5	50.2	842	96.67
20	13	118	18.2	50.9	903	91.32
103	14	64	27.4	54.6	583	99.42
13	15	57	21.8	53.2	684	92.20
28	16	29	22.2	53.6	292	118.85
98	17	32	25.3	51.9	604	94.41
127	18	92	22.3	54.1	847	96.67
89	19	38	21.8	54.3	720	94.41
163	20	95	22.1	60.8	554	103.80
110	21	51	24.7	53.2	792	96.24
5	22	25	23.4	54.1	348	118.85
11	23	114	16.5	48.0	968	91.32
87	24	67	22.9	51.0	700	92.20
66	25	76	24.7	59.8	316	124.44
38	26	29	23.0	53.2	390	120.85
63	27	124	21.7	55.2	302	123.99
48	28	171	23.0	58.1	682	97.34
70	29	51	27.5	54.5	505	99.42
37	30	35	27.3	56.0	245	126.65
65	31	32	27.2	51.1	310	126.65
127	32	121	22.4	57.2	636	96.67
116	33	114	23.9	56.2	356	123.99
20	34	127	18.6	51.6	820	91.32
71	35	108	28.8	65.3	553	102.22
123	36	99	26.6	61.0	340	110.53
127	37	102	24.2	54.6	640	96.67
15	38	51	28.8	58.1	239	128.68
38	39	25	23.6	54.5	332	120.85

Note: 1 mm = .0394 in., 1 MPa = 145 psi, 1 m³ = 1.308 yd³

proportions using approximate costs for each component material obtained from a local ready-mix concrete producer. Each of the four responses was analyzed by fitting a model, validating the model (by examining the residuals for trends and outliers), and interpreting the model graphically using contour and trace plots. The statistical analysis is described in detail for 28-day strength. The analyses for the other properties was performed in a similar manner.

Model Identification and Validation

The first step in the analysis is to identify a plausible model. Even though the design selected permits estimation of a quadratic model, a linear model may provide a better fit to the data. This is assessed using analysis of variance (ANOVA). The ANOVA results for 28-day strength are shown in Table 4^{6,7}. The row with source *linear* tests whether the

Table 4 – ANOVA Table for 28-day strength

Source	Sum of Squares	DOF	Mean Square	F Value	Prob > F
Mean	1.062E+05	1	1.062E+05		
Linear	257.52	5	51.50	5.46	0.0011
Quadratic	135.19	15	9.01	0.92	0.5665
Residual	147.62	15	9.84		
Total	1.068E+05	36	2965.37		

coefficients of the linear terms are equal. In the absence of quadratic terms, this means that mixing does not affect response (i.e., any mixture would give the same response). We conclude that the coefficients differ for low values (say less than 0.05) of the *Prob > F* (also called the p-value). Since the *Prob > F* value is 0.0011, we conclude that linear terms should be included in the model. The row with source *quadratic* tests whether any quadratic coefficients differ from zero. Since the *Prob > F* value of 0.5667 exceeds 0.05, we conclude that quadratic terms should not be included in the model.

The resulting linear model for 28-day strength (y_1), fit by least squares, is

$$\hat{y}_1 = -45.22x_1 + 89.15x_2 - 3.81x_3 + 1972x_4 + 38.36x_5 + 87.19x_6 \quad (7)$$

with residual standard deviation $s = 3.07$ MPa (445.4 psi).

The residual standard deviation s is defined as

$$s = \sqrt{\frac{\sum (y_i - \hat{y}_i)^2}{n-p}} \quad (8)$$

where the number of observations $n = 36$ and the number of parameters in the fitted model $p = 6$. A value of s near the repeatability value (replicate standard deviation) is an indication of an adequately fitting model. The repeatability value is 3.39 MPa (492.3 psi), which is close to s .

The fitted model is then validated by examining residual plots. The residuals are the deviations of the observed data from the fitted values, $y_i - \hat{y}_i$. The residual $y_i - \hat{y}_i$ estimates the error term e_i in the model. The e_i 's are assumed to be random and normally distributed with mean 0 and constant standard deviation. The residuals, which estimate these errors, should exhibit similar properties. Essentially, an adequate model should capture all information in the data leaving structureless, random residuals. If structure remains in the residuals, residual plots will often suggest how to modify the model to remove the structure. In this study, a plot of residuals versus run sequence as well as a plot of the control mix data revealed a linear trend in the data for each response. However, because the run sequence was randomized, this trend had little impact on the fitted models.

Graphical Interpretation

Once a valid model is obtained, it can be interpreted graphically using response trace plots and contour plots. A response trace plot is shown in Figure 4. This figure consists of six overlaid plots, one for each component. For a given component the fitted value of the response is plotted as the component is varied from its low to high setting in the constrained region, while the other components are held in the same relative ratio as a specified reference mixture, here the centroid. The plot shows the "effect" of changing each component on 28-day strength.

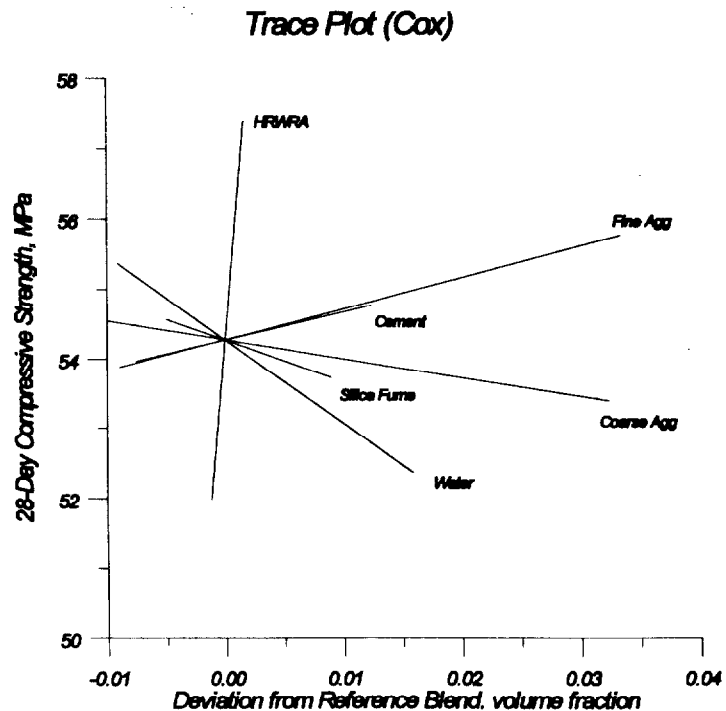


Figure 4. Trace plot for 28-day strength

As expected, increasing the amount of water decreased strength, while increasing the amount of cement increased strength. HRWRA had the largest effect with higher amounts of HRWRA yielding higher strength. This may be due to the improved dispersion of the cement and silica fume caused by higher amounts of HRWRA. Surprisingly, an increase in silica fume appears to reduce strength. This apparent reduction may not be significant when compared to the underlying experimental error.

Contour plots are used to identify conditions which give maximum (or minimum) response. Because contour plots can only show three components at a time (the others components are set at fixed conditions), several must be examined. Figure 5 is a contour plot of 28-day strength for water, cement, and HRWRA, with the other components fixed at their centroid values. The plot indicates that strength increases rapidly by increasing HRWRA, confirming the result from the response trace plot. Therefore, in subsequent

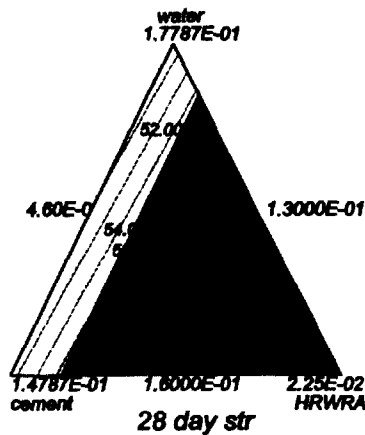


Figure 5. Contour plot for 28-day strength (MPa) in water, cement and HRWRA (microsilica = .018, CA = .410, FA = .259)

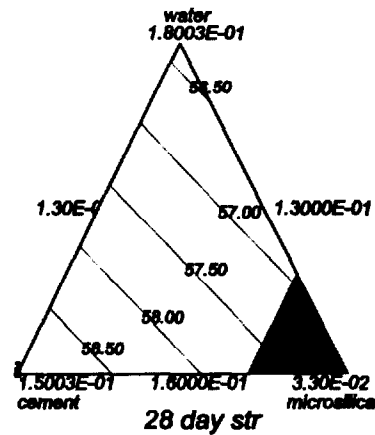


Figure 6. Contour plot for 28-day strength (MPa) in water, cement and microsilica (HRWRA = .0074, CA = .410, FA = .259)

contour plots, HRWRA will be set at its high value.

Figure 6 shows a contour plot of 28-day strength in water, cement, and microsilica, and Figure 7 shows a contour plot of 28-day strength in water, coarse aggregate, and fine aggregate. In each case, HRWRA is fixed at its high value and the other components are fixed at the centroid settings. These plots show that strength increases for low water, high cement, low microsilica, low coarse aggregate, and high fine aggregate. The best overall settings can be found using the contour plot shown in Figure 8 for microsilica, coarse aggregate, and fine aggregate at the best settings of water, cement, and HRWRA. The best settings (expressed as volume fractions) are water = 0.16, cement = 0.15, microsilica = 0.013, HRWRA = 0.0074, coarse aggregate = 0.40, and fine aggregate = 0.27, with a predicted value of strength of 59.53 MPa (8634 psi).

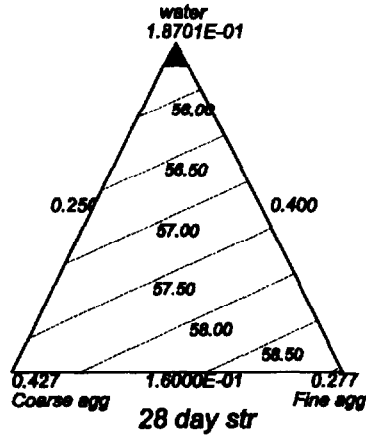


Figure 7. Contour plot for 28-day strength (MPa) in water, CA and FA (cement = .1376, microsilica = .018, HRWRA = .0074)

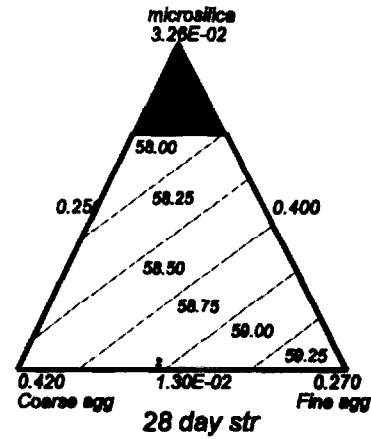


Figure 8. Contour plot for 28-day strength (MPa) in microsilica, fine aggregate, and coarse aggregate (water = .16, cement = .15, HRWRA = .0074)

Models for Other Responses

Using the same procedure described above for 28-day strength, the following models were fit to slump (y_2), 1-day strength (y_3), and 42-day RCT results (y_4):

$$\hat{y}_2 = 85.27x_1 - 94.09x_2 - 133.92x_3 + 955.63x_4 - 8.07x_5 + 6.69x_6 \quad (9)$$

$$\hat{y}_3 = -1.752E+05x_1 + 2.573E+05x_2 - 10723x_3 - 1.732E+06x_4 + 8632x_5 - 15245x_6 + 6.107E+05x_1x_6 - 8.118E+05x_2x_6 + 6.328E+06x_3x_4 + 6.481E+06x_4x_6 \quad (10)$$

$$\ln(\hat{y}_4) = 20.34x_1 - 2.99x_2 - 49.68x_3 - 29.65x_4 + 7.96x_5 + 4.15x_6 \quad (11)$$

Linear models were adequate for all responses except the 1-day strength, for which the fitted model includes four quadratic terms which were found to be significant. The natural logarithm of 42-day RCT was used for modeling, since residual plots showed that the standard deviation of 42-day RCT was proportional to the mean.

Selection of Optimum Mix

The optimum concrete mix is defined here as that mix which minimizes cost while meeting the specifications. Numerical optimization using desirability functions⁸ can be used to find the optimum mix. First, a desirability function must be defined for each property. The desirability function takes on values between 0 and 1, and may be defined in several ways, as indicated in Figure 9. Minimum and maximum specifications are used for strength and RCT, respectively, resulting in desirability functions with values of 1 above the minimum or below the maximum and zero otherwise. For example, for 1-day strength the desirability value is 0 below 22.06 MPa (3200 psi) and 1 above 22.06 MPa (3200 psi). At 34.48 MPa (5000 psi) the desirability becomes 0, however this strength was chosen to be well beyond the maximum value in the observed data. Desirabilities for 28-day strength and 42-day RCT are defined similarly. For slump a range of 50 to 100 mm (2 to 4 in) was specified, but the most desirable value is the midpoint of this range, or 75 mm (3 in). Therefore, the maximum desirability is given to the target value of 75 mm (3 in), with a linear decrease in desirability to a value of zero at the lower and upper specifications (see Figure 9). Since cost is to be minimized, the desirability function for cost decreases linearly over the range of costs observed in the data (see Figure 9). It is also possible to develop more complex desirability functions (e.g., non-linear function instead of linear for cost).

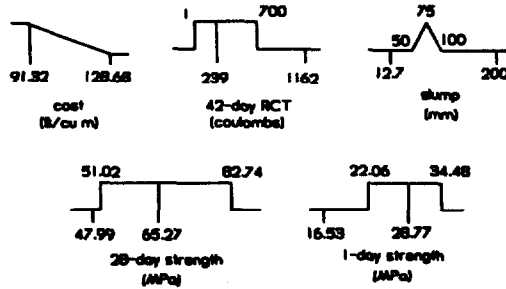


Figure 9. Desirability functions for optimization

In the numerical optimization scheme, the optimum mix maximizes the geometric mean D of the individual desirability functions d_i over the feasible region of mixtures, using the fitted models:

$$D = (d_1 d_2 d_3 d_4 d_5)^{1/5} \quad (12)$$

Based on the experimental results, the mix which maximizes D , expressed in volume fractions, is water = 0.160, cement = 0.130, microsilica = 0.013, HRWRA = 0.00493, coarse aggregate = 0.404, and fine aggregate = 0.287, at a cost of \$92.94 per cubic meter. The response values for this mix are slump = 75 mm (3 in), 1-day strength = 22.06 MPa (3200 psi), 28-day strength = 54.62 MPa (7922 psi), and 42-day RCT value = 653 coulombs.

If the fitted functions for each property were known without error, the analysis would be complete. However, there is uncertainty in the fitted functions since they are estimated from a sample of data. For example, at the current mix the predicted 1-day target strength is 22.06 ± 0.97 MPa (3200 ± 140 psi). The uncertainty provided is for a 95% confidence interval, i.e., we are 95% confident that the interval (21.09, 23.03) contains the true 1-day target strength for this mix. So if this mix is used, it is quite possible that the true 1-day target strength would fall below 22.06 MPa (3200 psi). Therefore, each specification must be modified to account for the uncertainty in the fitted function, which depends on the location of the mix in the feasible region. The uncertainties in the properties of the current mix can be used to modify the constraints and identify a revised optimal mix for these new constraints. The revised mix must then be checked to see that the specifications are met.

The predicted values and 95% uncertainties for the remaining responses at the current best mix are slump = 75 ± 15 mm (3.0 ± 0.6 in), 28-day strength = 54.62 ± 2.99 MPa (7922 ± 434 psi), and 28-day RCT = 653 ± 81 coulombs. The modified constraints on the responses which take into account the uncertainties are $66 \text{ mm} < \text{slump} < 86 \text{ mm}$ ($2.6 \text{ in} < \text{slump} < 3.4 \text{ in}$), 1-day target strength > 23.03 MPa (3340 psi), 28-day target strength > 53.78 MPa (7800 psi), and 42-day RCT < 620 coulombs. The best mix for this new set of constraints (expressed as volume fractions) is water = 0.160, cement = 0.135, microsilica = 0.0131, HRWRA = 0.00533, coarse aggregate = 0.401, and fine aggregate = 0.285 at a cost of \$72.54. The predicted values and 95% uncertainties for this mix are slump = 75 ± 15 mm (3 ± 0.6 in), 1-day strength = 23.09 ± 0.77 MPa (3349 ± 112 psi), 28-day strength = 55.48 ± 2.72 MPa (8047 ± 394 psi), and 42-day RCT = 617 ± 81 coulombs. The lower or upper bound values (as appropriate) for all responses meet the specifications.

CONCLUSIONS AND RECOMMENDATIONS

In high performance concretes consisting of many components, where several properties are of interest, it is critical to use a systematic approach for identifying optimal mixes given a set of constraints. Statistical experiment design and mixture experiments provide such an approach. They permit a thorough examination of a feasible region of interest in which to identify optimal mixes. Fitted models are obtained from the experimental data and are used to identify optimal mixes over the region.

Typically, quadratic models are assumed to provide an adequate representation of each property over the region of interest. For a six-component mixture, 21 mixes are required to fit a quadratic model, although additional runs should be included for checking the adequacy of the fitted model and estimating repeatability. A minimum of 31 runs is recommended. For the materials and conditions of this experiment, a linear model was adequate for all but one response (1-day strength). Since materials and conditions will vary by location, the quadratic model should be considered initially. However, if a linear model is found to be adequate for all responses of interest, the number of experimental runs can be halved.

Extra care is required to run a designed experiment; however, the results are well worth the additional effort. With many components and several properties of interest, trial and error methods could easily miss the optimal conditions, resulting in higher costs to producers over the long-term.

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